

Cyclohexane
110-82-7 | DTXSID4021923

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 91.3 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.80e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diethyl disulphide</div> <div>Measured: 96.9</div> <div>Predicted: 3.38</div>	<div>Image not found</div> <div>4-Butylphenol</div> <div>Measured: 76.2</div> <div>Predicted: 1.11e-02</div>	<div>Image not found</div> <div>1-Heptene</div> <div>Measured: 48.4</div> <div>Predicted: 57.8</div>
<div>Image not found</div> <div>Thietane</div> <div>Measured: 318</div> <div>Predicted: 31.0</div>	<div>Image not found</div> <div>Pentane, 1-fluoro-</div> <div>Measured: 59.3</div> <div>Predicted: 226</div>	